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Quantum Order: a Quantum Entanglement of Many Particles

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It is pointed out that quantum states, in general, contain a new kind of orders that cannot be characterized by symmetry. A concept of quantum order is introduced to describe such orders. As two concrete examples, we discussed quantum orders in free fermion systems and in 2D spin-1/2 systems. We generalize the Landau's theory for the classical orders and introduce projective symmetry group and Fermi surface topology to characterize different quantum orders.

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Introduction: Symmetry breaking and the associated order parameter have been playing a key role in our understanding of phases and phase transitions.[1, 2] However, recent study of quantum Hall (QH) liquids reveal that QH liquids contain a new kind of order – topological order – which can not be characterized by broken symmetry and the associated order parameter.[3, 4] Thus Landau's symmetry breaking theory for phase and phase transition does not apply to QH liquids and a new theory was developed to describe the topological orders in QH liquids.[5]

The reason that the Landau's symmetry breaking theory does not apply to QH liquids is because the Landau's theory was developed for classical statistical systems which are described by *positive* probability distribution functions of infinite variables. The QH liquids are described by their ground state wave functions which are *complex* functions of infinite variables. Thus it is not surprising that QH liquids contain addition structures (or a new kind of orders) that cannot be described by broken symmetries and the Landau's theory. From this point of view, we conclude that *any* quantum states may contain new kind of orders that are beyond broken symmetry characterization. Such kind of orders will be called quantum order.[6]

To visualize the distinction between the classical order and the quantum order, we may view the classical world described by positive probabilities as a "black and white" world, while the quantum world described by complex wave functions as a "colorful" world. The Landau's theory based on symmetry principle and order parameters is color blind which can only describe classical orders. We need to use new theories, such as the theory of topological/quantum orders, to characterize the rich "color" in quantum world. We can also view quantum order as a description of the pattern of the quantum entanglement in a many-body ground state. A special collective excitation above a quantum ordered state - gauge fluctuations - can be viewed as the fluctuations of quantum entanglement. In contract, the classical order in a crystal just describes a static positional pattern, which has no non-trivial quantum entanglement.

Quantum phase transitions and quantum orders: Classical orders can be studied through classical phase transitions. Classical phase transitions are marked by singularities in the free energy density f. The free energy density can be calculated through the partition function:

$$f = -\frac{T \ln Z}{V_{space}}, \quad Z = \int D\phi e^{-\beta \int dx h(\phi)} \qquad (1)$$

where $h(\phi)$ is the energy density of the classical system and V_{space} is the volume of space.

Similarly, to study quantum orders, we need to study quantum phase transition at zero temperature $T = 0$. Here the energy density of the ground state play the role of free energy density. A singularity in the ground state energy density marks a quantum transition. The similarity between the ground state energy density and the free energy density can be seen clearly in the following expression of the energy density of the ground state:

$$\rho_E = i\frac{\ln Z}{V_{spacetime}}, \quad Z = \int D\phi e^{i \int dx dt \mathcal{L}(\phi)} \qquad (2)$$

where $\mathcal{L}(\phi)$ is the Lagrangian density of the quantum system and $V_{spacetime}$ is the volume of space-time. We also note that the free energy density becomes the ground state energy density at $T = 0$. Comparing Eq. (1) and Eq. (2), we see that a classical system is described by a path integral of a positive functional, while a quantum system is described by a path integral of a complex functional. This is the real reason why the classical and quantum orders are different. According to the point of view of quantum order, a quantum phase transition, marked by a singularity of the path integral of a complex functional, in general, cannot be characterized by a change of symmetry and the associated order parameter. Thus, in general, we cannot use the broken symmetry and the Ginzburg-Landau theory to describe a continuous quantum transition.

Although the above discussion is limited to zero temperature, the path integrals of some quantum systems can be complex even at finite temperatures. Thus the above result also apply to quantum systems at finite temperatures. It is possible that a continuous phase tran-

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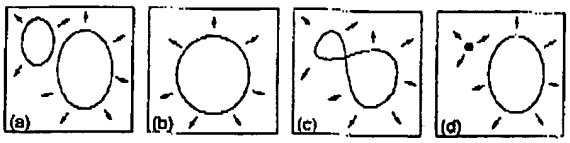

FIG. 1: Two sets of oriented Fermi surfaces in (a) and (b) represent two different quantum orders. The two possible transition points between the two quantum order (a) and (b) are described by the Fermi surfaces (c) and (d).

sition of a quantum system also does not involve any change of symmetry even at finite temperatures.

Quantum orders and quantum transitions in free fermion systems: Let us consider free fermion system with only the translation symmetry and the $U(1)$ symmetry from the fermion number conservation. The Hamiltonian has a form

$$H = \sum_{(ij)} \left(c_i^\dagger t_{ij} c_j + h.c. \right) \tag{3}$$

with $t_{ij}^* = t_{ji}$. The ground state is obtained by filling every negative energy state with one fermion. In general, the system contains several pieces of Fermi surfaces.

To understand the quantum order in the free fermion ground state, we note that the topology of the Fermi surfaces can changes in two ways as we continuously changing t_{ij}: (a) a Fermi surface shrinks to zero (Fig. 1d) and (b) two Fermi surfaces join (Fig. 1c). When a Fermi surface is about to disappear in a D-dimensional system, the ground state energy density has a form

$$\rho_E = \int \frac{d^D k}{(2\pi)^D} (k \cdot M \cdot k - \mu) \Theta(-k \cdot M \cdot k + \mu) + ...$$

where the ... represents non-singular contribution and the symmetric matrix M is positive (or negative) definite. We find that the ground state energy density has a singularity at $\mu = 0$: $\rho_E = c\mu^{(2+D)/2}\Theta(\mu) + ...$, where $\Theta(x > 0) = 1$, $\Theta(x < 0) = 0$. When two Fermi surfaces are about to join, the singularity is still determined by the above equation, but now M has both negative and positive eigenvalues. The ground state energy density has a singularity $\rho_E = c\mu^{(2+D)/2}\Theta(\mu) + ...$ when D is odd and $\rho_E = c\mu^{(2+D)/2} \log|\mu| + ...$ when D is even.

We find that the ground state energy density has a singularity at $\mu = 0$ which is exactly the same place where the topology of the Fermi surfaces has a change.[7] Thus the topology of the oriented Fermi surface is a "quantum number" that characterizes the quantum order in a free fermion system. (see Fig. 1). A change in the topology signals a *continuous* quantum phase transition. Lifshitz[7] also studied critical properties of such quantum transitions for $D = 3$.

Quantum order in spin liquids: Quantum order simply represents the quantum entanglement in ground state. The ground state wave function of a free fermion system has a simple form of Slater determinant. Its quantum order can be represented by the topology of the Fermi surfaces. In this section, we are going to discuss quantum orders in spin liquids. The ground state wave functions for spin liquids are more complicated and cannot be written as a Slater determinant. Thus we need to find a new way to characterize the quantum order in spin liquids.

The problem here is that the many-body wave function is too complicated to write down and it is hard to study them without writing them down. To gain some insights into the quantum entanglements in spin liquid states, in the following, we will discuss a concrete representation of the spin wave function. We will consider a spin-1/2 system on a 2D square lattice. For such a system, the spin wave function can be written as a bosonic wave function $\Phi(x_1, ..., x_{N_{up}})$, where x_i is the coordinate of the i^{th} up-spin and N_{up} is the total number of the up-spin.

Within the $SU(2)$ slave-boson approach,[8, 9] instead of writing down the bosonic wave function $\Phi(\{x_i\})$ directly, we regard the boson as a bound state of two fermions ψ_1 and ψ_2 (which will be called spinons) and write Φ as

$$\Phi(\{x_i\}) = \Psi_1(\{x_i\})\Psi_2(\{x_i\}) \tag{4}$$

where $\Psi_{1,2}$ are the wave functions of $\psi_{1,2}$ and have a form of Slater determinant.[10, 11] Actually, more general spin wave function can be constructed by introducing a mean-field Hamiltonian

$$H_{mean} = \sum_{ij} \psi_i^\dagger u_{ij} \psi_j + \sum_i \psi_i^\dagger a_0^l(i) \tau^l \psi_i \tag{5}$$

where $\psi^T = (\psi_1, \psi_2)$, $\tau^{1,2,3}$ are the Pauli matrices, and u_{ij} are 2×2 complex matrices. The collection $(u_{ij}, a_0^l \tau^l)$ is called a mean-field ansatz. For each mean-field ansatz, we can obtain a mean-field ground state by filling the lowest $2N_{up}$ energy levels of H_{mean} with the spinons ψ: $|\Psi_{mean}^{(u_{ij}, a_0^l \tau^l)}\rangle = \Psi_{mean}^{(u_{ij}, a_0^l \tau^l)}(y_1, .., z_1, ..)$, where y_i are the coordinates for ψ_1 and z_i for ψ_2. The physical spin wave function $\Phi(\{x_i\})$ can now be obtained by performing a projection[12] $y_i = z_i = x_i$:

$$\Phi^{(u_{ij}, a_0^l \tau^l)}(x_i) = |_{y_i = z_i = x_i} \Psi_{mean}^{(u_{ij}, a_0^l \tau^l)}(y_i, z_i) \tag{6}$$

Eq. (6) generalizes Eq. (4). What we have achieved here is that we manage to construct a large class of spin wave functions. Those spin wave functions Φ are related, through the projection, to the mean-field wave function Ψ which have a simple form of Slater determinant. The constructed spin wave function can be labeled by the mean-field ansatz $(u_{ij}, a_0^l \tau^l)$. This allows us to study the quantum order of a spin wave function by studying the property of a simpler object, the mean-field ansatz $(u_{ij}, a_0^l \tau^l)$.

In the study of phases and the related internal orders, the central question is to identify the universal properties of states. By definition, a universal property is a property

shared by all the states in the same phase. For classical systems, the symmetry of a state is a universal property. We cannot change one state to another state without a phase transition if the two states have different symmetries. Therefore, we can use the symmetry group (SG) to characterize the internal orders of classical states.

Similarly, to characterize quantum orders, we need to find the universal properties of spin liquid wave function. Using the above projective construction, we can simplify the problem by considering the universal properties of the mean-field ansatz $(u_{ij}, a_0^l\tau^l)$ instead. Motivated by the classical systems, here we would like to propose that the symmetry of the mean-field ansatz $(u_{ij}, a_0^l\tau^l)$ is a universal property. The symmetry group of the ansatz will be called the projective symmetry group (PSG). Under our conjecture, the quantum orders in spin liquids can be characterized by PSG's.

At the first sight, it appears that the PSG characterization of quantum orders is identical to the SG characterization of classical order used in Landau's theory. In fact the PSG of a spin wave function is different from the SG of that wave function and the two characterizations are different. This is because the $(u_{ij}, a_0^l\tau^l)$ labeling of the physical spin wave function $\Phi^{(u_{ij}, a_0^l\tau^l)}$ is not an one-to-one labeling. Two mean-field ansatz $(u_{ij}, a_0^l\tau^l)$ and $(\tilde{u}_{ij}, \tilde{a}_0^l\tau^l)$ differed by an $SU(2)$ gauge transformation defined by

$$\tilde{u}_{ij} = G(i)u_{ij}G^\dagger(j), \quad \tilde{a}_0^l(i)\tau^l = G(i)a_0^l(i)\tau^l G^\dagger(i),$$
$$\tilde{\psi}_i = G(i)\psi_i, \qquad G(i) \in SU(2) \tag{7}$$

give rise to the same spin wave function $\Phi^{(u_{ij}, a_0^l\tau^l)} = \Phi^{(\tilde{u}_{ij}, \tilde{a}_0^l\tau^l)}$. This is because the up-spin (the boson), as a bound state of ψ_1 and ψ_2, is an singlet of the above gauge $SU(2)$. Thus the spin wave function, as a projected mean-field wave function, is invariant under the local $SU(2)$ gauge transformation Eq. (7).

Due to the many-to-one labeling, an interesting situation appears. In order for a spin wave function to have a translation symmetry, its corresponding ansatz is only required to be translation invariant up to an $SU(2)$ gauge transformation. That is the ansatz should be invariant under translation followed by a proper gauge transformation. For example, to have a translation symmetry in x direction, u_{ij} should satisfy

$$u_{ij} = G_x T_x(u_{ij}), \quad a_0^l(i)\tau^l = G_x T_x(a_0^l(i)\tau^l);$$
$$T_x(u_{ij}) \equiv u_{i-\hat{x},j-\hat{x}}, \quad G_x(u_{ij}) \equiv G_x(i)u_{ij}G_x^\dagger(j) \tag{8}$$

for a certain $SU(2)$ gauge transformation $G_x(i)$. For two spin wave functions with the same translation symmetry, their ansatz can be invariant under translation followed by *different* gauge transformations. Thus two spin liquids with the same symmetry can have different PSG's. This indicates that the PSG characterization is more refined then the SG characterization. PSG can describe those internal structures that cannot be distinguished by SG. Therefore, we can use PSG to characterize quantum orders which cannot be completely characterized by symmetries.

Now let us explicitly write down PSG for some simple ansatz. We will consider spin liquids with *only* translation symmetry. The SG is generated by two translations in x and y directions $SG = \{T_x, T_y\}$. The first ansatz is called Z2A ansatz which has a form $u_{i,i+m} = u_m$, where $u_m = u_{-m}^\dagger$ are generic 2×2 complex matrices. An element in PSG, in general, is formed by the combined transformation as in Eq. (8). Including the translation in the y-direction, we find the PSG of the Z2A ansatz is generated by the following transformations $\{G_0, G_xT_x, G_yT_y\}$, where three gauge transformations G_0, G_x and G_y are given by $G_0(i) = -\tau^0$, $G_x(i) = \tau^0$, $G_y(i) = \tau^0$. Here τ^0 is the 2×2 identity matrix. Since the ansatz is already invariant under T_x and T_y, hence G_x and G_y are trivial.

We would like to point out that a PSG contains a special subgroup, which will be called the invariant gauge group (IGG). An IGG is formed by pure gauge transformations that leave the ansatz unchanged

$$IGG \equiv \{G|\ u_{ij} = G(i)u_{ij}G^\dagger(j), \qquad a_0^l(i)\tau^l = G(i)a_0^l(i)\tau^l G^\dagger(i)\} \tag{9}$$

One can show that PSG, IGG, and SG are related $PSG/IGG = SG$, thus comes the name projective symmetry group. For the Z2A ansatz, we find the IGG is a Z_2 group generated by $G_0 = -\tau^0$. Because of this we will call such a spin liquid a Z_2 spin liquid.

Next we consider another ansatz, the Z2B ansatz, $u_{i,i+m} = (-1)^{m_x i_y} u_m$. The Z2B PSG is still generated by $\{G_0, G_xT_x, G_yT_y\}$, but with a different G_y: $G_0(i) = -\tau^0$, $G_x(i) = \tau^0$, $G_y(i) = (-1)^{i_x}\tau^0$. Under translation T_y, $u_{i,i+m} \to u_{i-\hat{y},i+m-\hat{y}} = (-)^{m_x} u_{i,i+m}$. Thus we need a nontrivial gauge transformation $G_y = (-)^{i_x}$ to remove the extra factor $(-)^{m_x}$. The IGG for the Z2B ansatz, generated by G_0, is also Z_2 and the ansatz describes another Z_2 spin liquid.

One can show that[6] the above Z2A and Z2B PSG's cannot be transformed into each other by the $SU(2)$ gauge transformation Eq. (7). Therefore the Z2A and Z2B ansatz describe two spin liquids with the same symmetry but different quantum orders. This demonstrates that the ground state wave functions of spin liquids contain structures that cannot be characterized by symmetry. A generalization of the SG, PSG, can capture some of those extra structures.

To experimentally measure the different quantum orders in the Z2A and Z2B states, we can measure the spectrum of spin-1 excitations (*ie* the two-spinon excitations). One can show that (see Eq. (96) in Ref. [6]), for the Z2B state, the spin-1 spectrum is periodic in k-space with a period π in both x and y directions. For the Z2A state, the spin-1 spectrum has the usual period of 2π.

After constructing the spin wave functions of some spin liquids via the projection Eq. (6), we would like to ask: do those spin liquids actually exist for spin-1/2

systems? Are there any Hamiltonians such that the constructed spin wave functions are the ground state of those Hamiltonians? This is a very hard question and there are some recent work supporting the existence of spin liquids.[13, 14, 15, 16] It is also known that spin liquids do exist for certain large N systems.[17, 18, 19]. Here we would like to address an easier question about the stability of spin liquids: can a small perturbation in a spin Hamiltonian change the quantum order in the corresponding spin liquid. This question can be addressed without knowing the details of the lattice spin Hamiltonian. We only need to know the low lying spin excitations and their interactions.

As an example, we consider the stability of the Z2A spin liquid. Within the $SU(2)$ slave-boson mean-field theory,[8, 9] the spin excitations are described by the free spin-1/2 spinons ψ in the mean-field Hamiltonian Eq. (5). In general, if $|\mathrm{Tr}(u_m)|$ is much less then $|\mathrm{Tr}(u_m\tau^l)|$, the spinons have finite energy gap. As we go beyond the mean-field approximation, the low energy excitation also contain a collective mode described by the fluctuations δu_{ij}. The spinons are no longer free since they interact with δu_{ij}. As pointed out in Ref. [20], the fluctuations δu_{ij} correspond to a gauge field at low energies. The gauge group of the low energy gauge fluctuations is determined by the PSG.[6] In fact it is the IGG of the ansatz. (See also Ref. [17, 21, 22].) Thus the Z_2 spin liquid has a Z_2 gauge fluctuations at low energies. The Z_2 gauge fluctuations will cause an interaction between the spinons since they carry unit Z_2 charge. However, the Z_2 gauge interaction between the spinons is short ranged. Thus even beyond the mean-field theory, the spin 1/2 spinon excitations are free at low energies and the low energy gauge fluctuations do not cause any instability. All excitations, spinons and the Z_2 gauge fluctuations, have a finite energy gap. In this way, we showed that the Z2A spin liquid can be a stable spin liquid which represents a quantum phase. The low energy properties and the quantum order of the spin liquid do not change as we perturb the spin Hamiltonian.

In the above, we only showed that fluctuations around the Z_2 mean-field state do not cause any infrared divergence. However, even short distance fluctuations can cause instability if they are strong enough. Indeed the short distance fluctuations in our model are of order $O(1)$. This means that the projection Eq. (6) causes a big change and it is unclear if the projected state and the original state share similar physical properties. To make our approach here into a controlled calculation, we need to generalize our model to some large-N model. One way to do so is to generalize our mean-field Hamiltonian Eq. (5) to

$$H_{mean} = \sum_{ij} \psi^\dagger_{I,i} u_{ij} \psi_{I,j} + \sum_i \psi^\dagger_{I,i} a^l_0(i) \tau^l \psi_{I,i} \qquad (10)$$

where $I = 1, ..., N$ and we have N copies of two-component fields ψ_I. After integrating out the fermions, the effective Lagrangian for the fluctuations δu_{ij} has a form $\mathcal{L} = N\mathcal{L}_0(\delta u_{ij})$. In the large N limit, the fluctuations are suppressed and the mean-field theory becomes exact. Thus the two Z_2 states discussed above should exist in those large-N systems.

To obtain the physical system that corresponds to the mean-field theory Eq. (10), we note that a physical state must be a singlet of the gauge $SU(2)$ on every site. Thus the physical states on each site is formed by the singlet state of the fermions ψ_I. They include $|0\rangle$, $\psi^\dagger_{\alpha,I}\psi^\dagger_{\beta,J}\epsilon^{\alpha\beta}|0\rangle$, *etc* . The total number of physical state on each site is $N_p = \sum_{m=0}^{[N/2]} 2^{N-3m}(2m)!/m!$. Such a system is a system with N_p state per site (which can be viewed as a spin $S = (N_p-1)/2$ system without any spin rotation symmetry).

The PSG not only provides a concrete description of quantum order, it also allows us to partially classify quantum orders.[6] To understand the significance of PSG, we note that our understanding of solids is built on two corner stones: (A) Solids contain an order that is related to broken symmetry. (B) The order can be described and classified by SG's. In this paper we propose that a understanding of quantum phase should be built on (at least) the following two concepts: (A) A quantum phase in general contain a new kind of order - quantum order - which may not have broken symmetry and local order parameters. (B) The quantum order can be (partially) described and classified by PSG's.

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